III. Kinetic-Hydrodynamics Coupling

Kinetic and hydrodynamics equations

- Solving kinetic equations are much more expensive than solving hydrodynamic equations
- Defined in phase space (six dimension + time)
- More expensive when mean free path (Knudsen number=mfp/typical domain length)
 is small

Kinetic Equations (of monatomic gases)

$f_t + k \cdot \nabla_x f - \nabla_x V \cdot \nabla_k f = 1/\epsilon Q(f)$

f(t,x,k): probability density distribution

t: time x: position k: particle velocity

V(x): potential Q(f): collision operator

 ϵ : dimensionless mean free path or Knudsen number

Properties (for elastic collisions):

conservations of mass, moment and total energy;

H-theorem (entropy condition)

Scales in Kinetic (Boltzmann) Equations

- When ε is small (kn ≤ 0.01), the moments of f solve the compressive Euler (to leading order) or Navier-Stokes equations (to O(ε)) of fluid dynamics, except at initial, boundary or shock layers
- When ε is not small the fluid equations are not valid, so one has to use the kinetic equations

Multiscale Problems

- Very often one needs to deal with multiscale phenomena:
 - Space shuttle reentry $\epsilon: 10^{-8} \sim 1$ meters
 - fluid equations not accurate in boundary layers, shock layers, high Mach numbers
 - Different property of materials need different physical laws at different scales

Outline

Develop schemes that work uniformly with respect to ε:

asymptotic-preserving methods (kinetic schemes)

- Domain decomposition (hybridization method)
- Moment closure techniques

III-A: Asymptotic preserving methods

- Work in both kinetic and fluid regimes by solving only the kinetic equation; No need to couple two physical equations
- When ϵ is small, can do coarse (underresolved) computation: numerical discretization parameters (time step, mesh size) independent of ϵ
- Automatically become a fluid solver when $\epsilon \rightarrow 0$

Fluid approximations of kinetic equations

- The Euler scaling moments: ρ=∫ f dk mass ρ u = ∫ kf dk momentum E=1/2 ∫ |k|² f dk total energy
- when $\varepsilon \rightarrow 0$, Q(f) $\rightarrow 0$, then $f=\rho/(2\pi T)^{(d/2)} e^{-(k-u)^2/2T}=M$ local Maxwellian
- The moments ρ, ρ u, E solve the compressible Euler equations

High order approximations

- Chapman-Enskog expansion: expand in terms of power series of ε
- Zeroth order: Euler equations
- First order: Navier-Stokes equations
- Second order: Burnett equations (linearly unstable)
- Third order: super Burnett equations (linearly unstable)

Justifications of fluid dynamics limit (Caflish-Papanicolaou, Bardos-Golse-Levermore, Golse-Saint Raymond, ...)

Numerical issues when ϵ is small

- Numerical stiffness: an explicit collision term would require Δ t=O(ε)
- Implicit collision allows Δt to be independent of ε, but inverting the non-local collision term is numerically difficult and expensive
- Does the underresolved computation gives the correct macroscopic solutions?

Numerical goals

- Implicit collision that can be solved explicitly: underresolved time step; uniform stability
- Schemes capture the macroscopic behavior without resolving the small Knudsen number
- Asymptotic-preserving: numerical scheme should preserve the discrete analog of the Chapman-Enskog expansion

Asymptotic preserving



AP→Uniform convergence

• Golse-Jin-Levermore (SIAM J Num Anal 99)

For linear transport equation, with the diffusion limit, if the scheme is asymptotic-preserving, then

 $|| F^{\Delta}_{\epsilon} - f_{\epsilon} || \leq C (\Delta)^{n/2}$ Where C is independent of ϵ

Similar analysis applies to any other AP scheme

A case study-the BGK model

Coron-Perthame SINUM '91

•
$$f_t + k \cdot \nabla_x f = 1/\epsilon (M - f)$$

 $M = \rho/(2\pi T)^{(d/2)} e^{(k-u)/(2T)}$

Splitting:

 $\begin{array}{ll} \text{convection:} & f_t = 1/\epsilon \ (M-f) \\ \text{collision} & f_t + k \cdot \nabla_x \ f = 0 \end{array}$

Implicit collision

•
$$(f^{n+1}-f^n)/\Delta t = 1/\epsilon (M^{n+1}-f^{n+1})$$

Clearly $\Delta t=O(1)$

however, since elastic collision conserves ρ , u, T: Mⁿ⁺¹=M(ρ^{n+1} , uⁿ⁺¹, Tⁿ⁺¹)=M(ρ^{n+1} , uⁿ⁺¹, Tⁿ⁺¹)

Thus one can solve this implicit scheme explicitly!

This time discretization is AP: As \epsilon $\rightarrow 0$, fⁿ⁺¹ $\rightarrow M^{n+1}$, Plug this into the convection step gives the Euler equation

AP in space

- $\partial_t \mathbf{f} + \mathbf{k} \partial_x \mathbf{f} = \mathbf{0}$ using upwind: $\partial_t f_i + (k+|k|)/2 (f_i - f_{i-1}) / \Delta x$ + $(k-|k|)/2 (f_{i+1}-f_i) / \Delta x=0$ if one plugs f=M into the scheme, and take the moments, one arrives at
 - $\partial_t \mathbf{F} + [\mathbf{F}_{j+1/2} \mathbf{F}_{j-1/2}]/\Delta \mathbf{x} = \mathbf{0}$

• Where $F_{j+1/2} = F_{j+1/2}^+ = F_{j+1/2}^-$

$$\mathbf{F}_{i+\frac{1}{2}}^{-} = \rho_{i+\frac{1}{2}}^{-} \begin{pmatrix} \frac{v_{i+\frac{1}{2}}^{-}}{2} \mathcal{A}(-S_{i+\frac{1}{2}}^{-}) + \frac{1}{2} \frac{\mathcal{B}(S_{i+\frac{1}{2}}^{-})}{\sqrt{\pi\lambda_{i+\frac{1}{2}}^{-}}} \\ \begin{pmatrix} \left(\frac{v_{i+\frac{1}{2}}^{-}\right)^{2}}{2} + \frac{1}{4\lambda_{i+\frac{1}{2}}^{-}} \end{pmatrix} \mathcal{A}(-S_{i+\frac{1}{2}}^{-}) + \frac{v_{i+\frac{1}{2}}^{-}}{2} \frac{\mathcal{B}(S_{i+\frac{1}{2}}^{-})}{\sqrt{\pi\lambda_{i+\frac{1}{2}}^{-}}} \\ \begin{pmatrix} \left(\frac{v_{i+\frac{1}{2}}^{-}\right)^{3}}{4} + \frac{3}{8\lambda_{i+\frac{1}{2}}^{-}} v_{i+\frac{1}{2}}^{-} \end{pmatrix} \mathcal{A}(-S_{i+\frac{1}{2}}^{-}) + \begin{pmatrix} \left(\frac{v_{i+\frac{1}{2}}^{-}}{4} + \frac{1}{4\lambda_{i+\frac{1}{2}}^{-}} \right) \frac{\mathcal{B}(S_{i+\frac{1}{2}}^{-})}{\sqrt{\pi\lambda_{i+\frac{1}{2}}^{-}}} \end{pmatrix} \\ \end{pmatrix} \frac{\mathcal{B}(S_{i+\frac{1}{2}}^{-})}{\sqrt{\pi\lambda_{i+\frac{1}{2}}^{-}}} + \frac{1}{4\lambda_{i+\frac{1}{2}}^{-}} \frac{\mathcal{B}(S_{i+\frac{1}{2}}^{-})}{\sqrt{\pi\lambda_{i+\frac{1}{2}}^{-}}} \end{pmatrix} \frac{\mathcal{B}(S_{i+\frac{1}{2}}^{-})}{\sqrt{\pi\lambda_{i+\frac{1}{2}}^{-}}} \end{pmatrix}$$

and

$$\mathbf{F}_{i+\frac{1}{2}}^{+} = \rho_{i+\frac{1}{2}}^{+} \begin{pmatrix} \frac{v_{i+\frac{1}{2}}^{t}}{2} \mathcal{A}(S_{i+\frac{1}{2}}^{+}) - \frac{1}{2} \frac{\mathcal{B}(S_{i+\frac{1}{2}}^{+})}{\sqrt{\pi\lambda_{i+\frac{1}{2}}^{-}}} \\ \begin{pmatrix} \frac{(v_{i+\frac{1}{2}}^{+})^{2}}{2} + \frac{1}{4\lambda_{i+\frac{1}{2}}^{+}} \end{pmatrix} \mathcal{A}(S_{i+\frac{1}{2}}^{+}) - \frac{v_{i+\frac{1}{2}}^{-}}{2} \frac{\mathcal{B}(S_{i+\frac{1}{2}}^{+})}{\sqrt{\pi\lambda_{i+\frac{1}{2}}^{+}}} \\ \begin{pmatrix} \frac{(v_{i+\frac{1}{2}}^{+})^{2}}{4} + \frac{3}{8\lambda_{i+\frac{1}{2}}^{+}} v_{i+\frac{1}{2}}^{+} \end{pmatrix} \mathcal{A}(S_{i+\frac{1}{2}}^{+}) - \begin{pmatrix} \frac{(v_{i+\frac{1}{2}}^{+})^{2}}{4} + \frac{1}{4\lambda_{i+\frac{1}{2}}^{+}} \end{pmatrix} \frac{\mathcal{B}(S_{i+\frac{1}{2}}^{+})}{\sqrt{\pi\lambda_{i+\frac{1}{2}}^{+}}} \end{pmatrix},$$

where

$$A(S) = \operatorname{erfc}(S), \quad B(S) = \exp(-S^2), \quad S^{\pm} = v^{\pm}\sqrt{\lambda^{\pm}}, \quad \lambda = \frac{1}{2\theta},$$

This is the kinetic flux vector splitting scheme for compressible Euler by Deshpande

More general collision terms

 using the Wild sum for more general collision operators

(Gabette, Pareschi, Toscani, SIAM J Num Anal '97)

High order time discreitzations

- second order Strang splitting reduces to first order as \epsilon→0:
 - * Jin, J. Comp. Phys. 95
- usually L-stable ODE solvers work:
 - * Runge-Kutta splitting: *Caflish, Jin, Russo*, SIAM J. Num Anal. 97
 - * Implicit-Explicit (IMEX) time discretizations: *Pareschi-Russo,*

(Incompressible) Navier-Stokes or diffusive limit

• Transport equation in the diffusive regime

$$\epsilon \, \partial_t f + \mathbf{v} \cdot \nabla_x f = \frac{1}{\epsilon} \left[\frac{\sigma_s}{S} \int_\Omega f d\mathbf{v}' - \sigma f \right] + \epsilon Q,$$

• The diffusion limit: as $\varepsilon \rightarrow 0$, f $\rightarrow \rho^{(0)}$, where

$$\partial_t \rho^{(0)} = D \nabla_x \cdot \left(\frac{1}{\sigma} \nabla_x \rho^{(0)} \right) - \sigma_A \rho^{(0)} + Q,$$

An AP scheme (J-Pareschi-Toscani, SINUM '00)

Split this equation as two equations, each for v > 0:

(3.2)

$$\begin{aligned} \epsilon \partial_t f(v) + v \partial_x f(v) &= \frac{1}{\epsilon} \left(\frac{1}{2} \int_{-1}^1 f dv - f(v) \right), \\ \epsilon \partial_t f(-v) - v \partial_x f(-v) &= \frac{1}{\epsilon} \left(\frac{1}{2} \int_{-1}^1 f dv - f(-v) \right). \end{aligned}$$

In this case the even- and odd-parities are

$$r(t, x, v) = \frac{1}{2} [f(t, x, v) + f(t, x, -v)],$$

$$j(t, x, v) = \frac{1}{2\epsilon} [f(t, x, v) - f(t, x, -v)].$$

Adding and subtracting the two equations in (3.2) lead to

(3.3)
$$\partial_t r + v \partial_x j = \frac{1}{\epsilon^2} (\rho - r),$$
$$\partial_t j + \frac{v}{\epsilon^2} \partial_x r = -\frac{1}{\epsilon^2} j,$$

An AP scheme (cont'd)

• Solve the relaxation step (by some L-stable implicit ODE solver)

$$\begin{split} \partial_t r &= -\frac{1}{\epsilon^2} \left(r - \rho \right), \\ \partial_t j &= -\frac{1}{\epsilon^2} \left(j + (1 - \epsilon^2 \phi) v \partial_x r \right), \end{split}$$

• Solve the convection step (by some explicit shock capturing scheme)

$$\partial_t r + v \partial_x j = 0,$$

 $\partial_t j + \phi v \partial_x r = 0.$

Here $\phi(\varepsilon)$ =min {1, 1/ ε } is a front wave speed

(related work: *Klar*)

Numerical example: transport to diffusion



Jin, Pareschi, Toscani: SIAM J. Num Anal. '00

Numerical example: transport to diffusion



Jin, Pareschi, Toscani: SIAM J. Num Anal. '00



Two space dimension



Other AP schemes

- A. Klar
- Carrillo-Goudon
- Lemou-Mieussens
- Hauck-Lowrie
- Degond etc. for plasma (Euler-Poisson, Valsov-Poisson)
- Asymptotic-preserving Monte Carlo
 Caflish-Pareschi-Russo '99--

III-B: Domain decomposition methods



Different couplings

• Artifical interface:

* add an artificial interface to couple a kinetic and hydrodynamic equations

*where should the interface be?

 Physical interface need physical interface condition, interface layer

Artifical coupling: Previous works

sharp interface coupling:

- Bouygat-Mallinger-Le Tallec-Tidriri,
- Klar-Neunzert
- Perthame-Qiu

can be easily implemented if kinetic schemes are used for hydrodynamics

Difficulty: where to put the interface

A sharp interface coupling



A smooth transition model

- *Degond-Jin*: SIAM J. Num. Anal. 05
- Degond-Jin-Mieussens: J. Comp. Phys. 05



Kinetic/kinetic coupling

$$\partial_t f + v \partial_x f = Q(f) \qquad -\infty < \mathbf{X} < \infty \qquad (1)$$

If we define the two distributions $f_L^{\varepsilon} = h f^{\varepsilon}$ and $f_R^{\varepsilon} = (1 - h) f^{\varepsilon}$, then it is easy be check that they satisfy the following coupled system:

$$\partial_t f_L^{\varepsilon} + h v \partial_x f_L^{\varepsilon} + h v \partial_x f_R^{\varepsilon} = \frac{1}{\varepsilon} h Q (f_L^{\varepsilon} + f_R^{\varepsilon}), \tag{6}$$

$$\partial_t f_R^{\varepsilon} + (1-h)v \partial_x f_R^{\varepsilon} + (1-h)v \partial_x f_L^{\varepsilon} = \frac{1}{\varepsilon} (1-h)Q(f_L^{\varepsilon} + f_R^{\varepsilon}), \tag{7}$$

with initial data

$$f_L^{\varepsilon}|_{t=0} = h f_0, \qquad f_R^{\varepsilon}|_{t=0} = (1-h) f_0.$$
 (8)

The hydrodynamic limit

- When ε→0, f^ε → E[ρ], where ρ(t,x) is a solution to the hydrodynamic equation
 ∂_t ρ +∂_x F(ρ)=0
 - ρ : hydrodynamic variables F(ρ): the hydrodynamic flux F(ρ)=<vmF(ρ)>

The hydrodynamic limit of f_R^{ϵ}

• When $\varepsilon \rightarrow 0$, $f_{R}^{\varepsilon} \rightarrow F(\rho_{R}^{\varepsilon})$, where ρ_{R}^{ε} is a solution to the hydrodynamic equation

 $\partial_t \rho^{\epsilon}_{R}$ +(1-h) F(ρ^{ϵ}_{R})+(1-h)<vmf^{\epsilon}_{L}>=0

Kinetic/hydrodynamic coupling

$$\begin{split} \partial_t f_L^\varepsilon + hv \partial_x f_L^\varepsilon + hv \partial_x E[\rho_R^\varepsilon] &= \frac{1}{\varepsilon} hQ(f_L + E[\rho_R^\varepsilon]), \\ \partial_t \rho_R^\varepsilon + (1-h) \partial_x F(\rho_R^\varepsilon) + (1-h) \partial_x \langle vm f_L^\varepsilon \rangle = 0, \end{split}$$

 $f_L^{\varepsilon}|_{t=0} = hf_0, \quad \rho_R^{\varepsilon}|_{t=0} = (1-h)\rho_0.$ $\mathbf{f}^{\varepsilon} = \mathbf{f}^{\varepsilon}_{\mathsf{L}} + \mathbf{E}(\boldsymbol{\rho}^{\varepsilon}_{\mathsf{R}})$

Remark: no boundary condition is needed since the equation is degenerate at x=(a+b)/2: h=0

Conditions/constraints

- General geometry of the interface has been built into the h-function
- The mapping $\rho \rightarrow E(\rho)$ should be homogeneous of degree one E($\lambda \rho$)= $\lambda E(\rho)$ for any λ >0
- Classical kinetic models for rarified gas or plamsa (Boltzmann, BGK, Fokker-Planck-Laudau) OK:

$$E[\rho] = \frac{n}{(2\pi\theta)^{1/2}} \exp\left(-\frac{(v-u)^2}{2\theta}\right).$$

 Quantum kinetic models with Fermi-Dirac or Bose- Einstein statistics not OK:

$$E[\rho] = \frac{1}{\exp(\frac{\epsilon - \mu}{\tau}) \pm 1}$$
 (+ Fermi-Dirac, - Bose-Einstein).

- Constraints can be removed using micro-macro decomposition $f=E(\rho)+g$

(Degond-Liu-Mieussens)

1d numerical example: shock tube

- Solid line: coupling method
- Dot line: BGK
- Dash-dot: Euler





Shock defraction around a circular cylinder (Kn=0.005, Mach=2.81)



6

Physical interface

• Due to different materials, one needs to couple equations at different scales via a physical interface boundary condition

Transport/diffusion coupling



approaches

- f₊ can not be directly used for diffusion boundary condition: a boundary (interface) condition based on matched boundary layer analysis is needed to derive the boundary condition for the diffusion equation
- A reflecting boundary condition at x_M can be used for the transport equation

Different physical interfaces

 Density (energy) conserved at interface Golse-Jin-Levermore, M2AN '03

 Density (energy) flux conserved at interface Bal-Ryzhik derived interface condition Jin-Yang-Yuan: domain decomposition method allow partial specular or diffusive transmission/reflection

III-C: Moment Methods

multiply the Boltzmann equation by the functions $\phi_i(k)$ (i=1, ..., N, ...)

$$\begin{array}{ll} \partial_t \int \phi_i(k) \; f(t,\,x,\,k) \; \; dk + \nabla \cdot \int \; \phi_i(k) \; k \; f(t,\,x,\,k) \; \; dk \\ &= \int \phi_i(k) \; Q(f) \; dk \qquad \quad i=1,\;\cdots,\;N,\;\cdots \end{array}$$

how to close the system with finite many moments:

- Grad's thirteen moments (density, momentum, energy, stress, heat flux): f is a Maxwellian times a Hermite function of k
- Muller: Extended Thermodynamics: using more moments

look for models for transition regimes (0.01 \leq Kn \leq 1)

Better Hydrodynamic Models?

The Navier-Stokes equations are not valid in rarefied gas (high altitude flights, microscopic flows, etc.) or inaccurate in shock and boundary layers

If one does not want to go back to Boltzmann, then intermediate models are desired.

- improved constitutive relation
- use more moments.

Disadvantage of the Moment Methods

- work well for low Mach number flow (Ma \leq 1.6)
- For higher Mach number flow it gives unphysical
 sub-shocks
 - elliptic region
 - deviate from the experiments and Monte Carlo results across the shock layer.
- Including higher moments eventually cure this problem but one needs many moments and the increase in Mach number is very slow

Chapman-Enskog expansion

Constitutive relation for ideal gas: μ --viscosity

T= -p I- P, p =R $\rho\theta$, P= $\mu \Pi^{(1)} + \mu^2 \Pi^{(2)} + \mu^3 \Pi^{(3)} + \cdots$, q = $\mu \Xi^{(1)} + \mu^2 \Xi^{(2)} + \mu^3 \Xi^{(3)} + \cdots$

O(1): Euler

- O(µ): Navier-Stokes equations
- $O(\mu^2)$: Burnett equations
- $O(\mu^3)$: super Burnett equations

About Burnett equations

- linearly unstable: inconsistent to the second law of thermodynamics
- going to higher order does not help
- give more accurate shock profile for hypersonic flow than the Navier-Stokes equations when compared with the Direct Simulation Mont Carlo (*Fiscko-Chapman, '88 Agarwal, '00*)

Relaxed Burnett equations

- Jin-Slemrod (J. Stat. Phys. '91)
- a relaxation scheme to regularize the Burnett equations
- defining the Stress and Heat Flux (thus the constitutive relation) with rate equations as in visco-elastic fluids.
- This gives a system of thirteen equations
- linearly stable
- Has a globally defined nonlinear entropy function that is consistent to the Second Law of Thermodynamics
- Chapman-Enskog expansion shows it agrees with the Boltzmann equation to the Burnett (second) order,

A model problem

$$u_t = \varepsilon \ u_{xx} - \varepsilon^2 \ u_{xxt}$$

Here the second order term resembles N-S viscosity while the third order term is that of Burnett approximation

Fourier Transform on x gives

$$U_t = -ε ξ^2/(1-ε^2 ξ^2) U$$

this is a high-frequency instability if

A relaxation model

Consider the following "hyperbolic heat" equation

$$\begin{cases} u_t + \epsilon q_x = 0 \\ q_t + 1/\epsilon u_x = -1/\epsilon q \end{cases}$$

This is a hyperbolic system with a relaxation, which is endowed with a convex entropy $u^2/+\epsilon^2 q^2$

Chapman-Enslog expansion

- $q=-U_x \varepsilon q_t$ = $-u_x + \varepsilon u_{x+} + O(\varepsilon^2)$ Applying this to $u_t+q_x=0$ Gives $u_t = \varepsilon u_{xx} - \varepsilon^2 u_{xxt}$
 - Our idea is to use the first-order "good" relaxation system, rather than the third order "unstable" Burnett equation

Relaxed Burnett equation

 $\dot{\rho} + \rho \text{ div } \mathbf{u} = 0,$ $\rho \dot{\mathbf{u}} + \text{grad } p + \text{div } \mathbf{P} = \rho \mathbf{b},$

 $\mathbf{P}=\mathbf{P}^T,$

$$\dot{\mathbf{P}} - \mathbf{L}\mathbf{P} - \mathbf{P}\mathbf{L}^{T} + \frac{2}{3}\mathrm{tr}(\mathbf{P}\mathbf{L}^{T})\mathbf{I} = -\frac{2p}{\omega_{2}\mu}\left(\mathbf{P} - \mathbf{P}^{eq}\right),$$
$$\rho\dot{\mathbf{e}} + p \,\operatorname{div}\,\mathbf{u} + \mathbf{P} \cdot \mathbf{S} + \operatorname{div}\,\mathbf{q} = 0,$$
$$\dot{\mathbf{q}} - \mathbf{L}^{T}\mathbf{q} = -\frac{3Mp}{2\theta_{2}\mu}\left(\mathbf{q} - \mathbf{q}^{eq}\right),$$

$$\mathbf{P}^{eq} = -2\mu\mathbf{S} + \mathbf{P}_2 + \mathbf{P}_3,$$

$$\begin{split} \mathbf{P}_{2} &= -\mu \frac{\omega_{1}}{2p} (\operatorname{divu}) \mathbf{P} + \frac{\omega_{2} \mu'(\theta) \dot{\theta}}{2p} \mathbf{P} \\ &+ \mu^{2} \frac{\omega_{3}}{\rho \theta} \left\{ -\operatorname{grad} \left(\frac{\mathbf{q}}{\frac{3}{2} \mu M R} \right) + \frac{1}{3} \operatorname{div} \left(\frac{\mathbf{q}}{\frac{3}{2} \mu M R} \right) \mathbf{I} \right\} \\ &+ \mu \frac{\omega_{4}}{\rho \rho \theta} \left\{ -\frac{1}{2} \operatorname{grad} p \otimes \left(\frac{\mathbf{q}}{\frac{3}{2} M R} \right) - \frac{1}{2} \left(\frac{\mathbf{q}}{\frac{3}{2} M R} \right) \otimes \operatorname{grad} p \\ &+ \frac{1}{3} \operatorname{grad} p \cdot \left(\frac{\mathbf{q}}{\frac{3}{2} M R} \right) \mathbf{I} \right\} \\ &- \mu \frac{\omega_{5}}{\rho \theta^{2}} \left\{ \frac{1}{2} \operatorname{grad} \theta \otimes \left(\frac{\mathbf{q}}{\frac{3}{2} M R} \right) + \frac{1}{2} \left(\frac{\mathbf{q}}{\frac{3}{2} M R} \right) \otimes \operatorname{grad} \theta \\ &- \frac{1}{3} \operatorname{grad} \theta \cdot \left(\frac{\mathbf{q}}{\frac{3}{2} M R} \right) \mathbf{I} \right\} - \mu \frac{\omega_{6}}{2p} \left\{ \frac{1}{2} (\mathbf{SP} + \mathbf{PS}) - \frac{1}{3} \operatorname{tr}(\mathbf{PS}) \mathbf{I} \right\}, \\ \mathbf{P}_{3} &= \mu^{2} \left[\frac{\omega_{2}}{p^{2}} \operatorname{tr} \mathbf{S}^{2} + \omega_{3} \frac{|\operatorname{grad} \theta|^{2}}{R \rho^{2} \theta^{3}} \right] \mathbf{P} + \mu \frac{\gamma_{1}}{p \theta} \left(\dot{\theta} + \frac{2}{3} \theta \operatorname{div} \mathbf{u} \right) \mathbf{P} \\ &+ \omega_{4} \left[\frac{\mu^{3}}{M R \rho^{2}} \left(\frac{1}{2 \mu \theta} P^{ij} \right)_{,k} \right]_{,k}, \\ \mathbf{q}^{eq} &= -\frac{3}{2} \mu M R \operatorname{grad} \theta + \mathbf{q}_{2} + \mathbf{q}_{3}, \\ \mathbf{q}_{2} &= -2 \mu \frac{\theta_{1}}{3M R \rho \theta} (\operatorname{div} \mathbf{u}) \mathbf{q} + \frac{2 \theta_{2} \dot{\theta} \dot{\mu}'(\theta)}{3M R \rho \theta} \mathbf{q} \\ &- \mu \frac{\theta_{3}}{2 p \rho} \mathbf{P} \operatorname{grad} p - \mu^{2} \frac{\theta_{4}}{2 \rho} \operatorname{div} \left(\frac{\mathbf{P}}{\mu} \right) - \mu \frac{\theta_{5}}{2 \rho \theta} \mathbf{P} \operatorname{grad} \theta, \\ \mathbf{q}_{3} &= \mu^{2} \left[\frac{\hat{\theta}_{2}}{p^{2}} \operatorname{tr} \mathbf{S}^{2} + \hat{\theta}_{3} \frac{|\operatorname{grad} \theta|^{2}}{R \rho^{2} \theta^{3}} \right] \mathbf{q} + \mu \frac{\hat{\lambda}_{1}}{\rho \theta^{2}} \left(\dot{\theta} + \frac{2}{3} \theta \operatorname{div} \mathbf{u} \right) \left(\frac{\frac{\mathbf{q}}{\frac{3}{2} M R} \right) \\ &+ \hat{\theta}_{4} \left[\frac{\mu^{3} \theta}{\rho^{2}} \left(\frac{2}{3M R \mu \theta^{2}} q_{i} \right)_{,k} \right]_{,k}. \end{split}$$

A stationary, Mach TU Shock



Numerical observations

- For small Mach numbers (\leq 1.6) all these methods give comparable results
- Relaxed Burnett offers more accurate shock profiles for larger Mach numbers, the larger the better
- Also extended to granular flow (Jin-Slemrod Physica D '01)

Other transition models

- Levermore
- R13
 - H. Struchtrup:

Macroscopic Transport Equations for Rarefied Gas Flows: Approximation Methods in Kinetic Theory, Springer 2005

Summary

- Three methods were discussed for multiscale kinetic problems:
- asymptotic-preserving: solving one equation (kinetic), more efficiency in the fluid regime; don't use hydrodynamic equations – good when they are not available
- domain decomposition: more efficient than AP, but trickier at the interface
- moment methods: for transition regime, most efficient, but no perfect models (stability+entropy+accuracy)